Clay-fulleropyrrolidine nanocomposites

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Supporting Information

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Cartesian Coordinates of the clay layer used in the simulations

1	Si	1.163127	1.654734	-3.014514	160
2	O	2.734203	1.777204	-3.462397	163
3	O	1.216158	1.840217	-1.340980	163
4	Si	3.543532	5.881427	-2.746584	160
5	Al	2.507178	7.301720	-0.013279	161
6	O	3.083359	4.316824	-3.004541	163
7	O	5.064331	6.168889	-3.275046	163
8	O	3.477761	5.996230	-1.072394	163
9	O	0.784246	4.455705	-1.074598	163
10	H	1.664815	4.460617	-1.164023	166
11	Si	3.765841	2.832241	-2.716443	160
12	Al	2.599116	1.463700	0.010837	161
13	O	5.296831	2.538175	-3.224038	163
14	O	3.748967	2.646147	-1.042615	163
15	O	0.499807	8.843513	-3.286691	163
16	Al	5.261982	2.841305	0.090461	161
17	O	3.354819	8.827715	-0.968496	163
18	H	4.224180	8.911511	-0.822651	166
19	O	1.659742	8.843849	0.930131	163
20	H	0.830908	8.911718	0.625649	166
21	Si	4.035292	1.389899	3.017072	160
22	O	2.503397	1.801994	3.417015	163
23	O	4.132324	1.437424	1.320936	163
24	O	4.535534	8.828370	3.222312	163
25	Si	4.062619	7.299484	2.856365	160
26	Al	5.046240	5.851897	0.107070	161
27	O	2.498821	7.078624	3.422497	163
28	O	4.037449	7.117696	1.194862	163
29	Si	0.949564	7.321338	-2.878263	160
30	O	2.488618	6.974608	-3.401370	163
31	O	0.944287	7.190626	-1.203045	163
32	Na	1.463548	8.870363	5.179714	164
33	Si	1.483494	5.932821	2.738468	160
34	O	2.015752	4.415977	3.081928	163

35	O	-0.040954	6.232180	3.268729	163
36	O	1.516332	6.066669	1.078442	163
37	O	4.299521	4.287067	1.051912	163
38	H	3.422729	4.166572	1.071600	166
39	Si	1.471349	2.887646	2.744130	160
40	O	-0.066351	2.570875	3.206279	163
41	O	1.610573	2.764247	1.062681	163
42	Si	0.957705	10.351334	-2.827066	160
43	O	2.488891	10.627410	-3.417058	163
44	O	0.969715	10.513817	-1.154984	163
45	Si	3.616452	14.815165	-2.843990	160
46	Mg	2.629637	16.091941	0.014957	168
47	O	3.025318	13.307726	-3.190048	163
48	O	5.138797	15.091519	-3.405526	163
49	O	3.652781	14.879521	-1.168468	163
50	O	0.794066	13.325089	-1.008988	163
51	H	1.678582	13.306850	-1.038106	166
52	Si	3.531897	11.780069	-2.841583	160
53	Al	2.513974	10.393647	-0.018696	161
54	O	5.037823	11.451652	-3.409979	163
55	O	3.498110	11.649965	-1.161859	163
56	O	0.478305	17.766502	-3.195611	163
57	Al	5.061449	11.781406	0.020400	161
58	O	3.442841	17.754869	-0.970046	163
59	H	3.911923	17.179036	-0.487403	166
60	O	1.813293	17.754082	0.998383	163
61	H	1.359059	17.184840	0.493983	166
62	Si	4.080627	10.345769	2.775740	160
63	O	2.532847	10.553123	3.394721	163
64	O	4.038208	10.527141	1.116579	163
65	O	4.696882	17.767751	3.194426	163
66	Si	4.158326	16.270579	2.730951	160
67	Al	5.210622	14.801659	-0.047138	161
68	O	2.662604	15.937783	3.306474	163
69	O	4.318230	16.183872	1.056278	163
70	Si	1.058057	16.282728	-2.687251	160
71	O	2.549464	15.985711	-3.293227	163
72	O	0.940886	16.194533	-1.018843	163
73	Si	1.599646	14.771446	2.849705	160
74	O	2.098420	13.236458	3.209343	163
75	O	0.085164	15.075161	3.412142	163
76	O	1.616796	14.820795	1.167698	163
77	O	4.292991	13.356646	0.972662	163
78	H	3.450931	13.619187	0.893028	166
79	Si	1.532870	11.754994	2.787316	160
80	O	0.028165	11.421082	3.379705	163
81	O	1.518919	11.613083	1.122470	163